

Mott transition and dimerization in the one-dimensional $SU(n)$ Hubbard model

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The one-dimensional $SU(n)$ Hubbard model is investigated numerically for $n = 2, 3, 4$, and 5 at half filling and $1/n$ filling using the density-matrix renormalization-group (DMRG) method. The energy gaps and various quantum information entropies are calculated. In the half-filled case, finite spin and charge gaps are found for arbitrary positive U if $n > 2$. Furthermore, it is shown that the transition to the gapped phase at $U_c = 0$ is of Kosterlitz-Thouless type and is accompanied by a bond dimerization both for even and odd n . In the $1/n$ -filled case, the transition has similar features as the metal-insulator transition in the half-filled $SU(2)$ Hubbard model. The charge gap opens exponentially slowly for $U > U_c = 0$, the spin sector remains gapless, and the ground state is non-dimerized.

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I. INTRODUCTION

Recently, the $SU(n)$ -symmetric generalization of the standard $SU(2)$ Hubbard model¹ has been intensively studied theoretically,^{2,3,4,5,6,7,8} since this model may mimic strongly correlated electron systems where the orbital degrees of freedom of d and f electrons play important role.

Although the standard $SU(2)$ Hubbard model is exactly solvable in one dimension⁹ by Bethe's ansatz and is well known to exhibit—at half filling—a Mott transition at $U_c = 0$, no such rigorous statement could be formulated for higher n values. It is expected, however, that at generic fillings the one-dimensional $SU(n)$ Hubbard model behaves like an n -component Luttinger liquid while gaps may be generated at special fillings of the band, namely at half filling or $1/n$ filling.

The one-dimensional half-filled $SU(n)$ Hubbard model has been studied² in the large n limit and it has been shown that the charge and spin modes—that are decoupled for $n = 2$ —become coupled and gap is generated in all of them. Moreover, it has been found that the system is spontaneously dimerized if n is even. The role of umklapp processes in the half-filled model has been studied⁷ by the analytic multiplicative renormalization-group method in fermionic representation, too. It has been shown that in fact the umklapp processes couple the spin and charge modes if $n > 2$ and the spectrum is fully gapped for arbitrary values of the Coulomb repulsion. The question of dimerization has not been addressed in that work.

The $1/n$ -filled case has been investigated³ analytically using the bosonized version of the model and numerically with quantum Monte Carlo simulation. It has been shown that at this special filling, i.e., when the number of particles is equal to the number of sites, the spin and charge degrees of freedom are decoupled and gap opens in the charge mode only. The spin modes remain gapless. Furthermore, it was inferred from the numerical calculations that for $n > 2$, unlike in the $n = 2$ case, the charge gap opens at a finite positive U_c . For smaller positive

U values the system shows metallic behavior. Since the contributions of the leading umklapp processes for commensurate fillings—except for half filling—are not logarithmically divergent, the special case of $1/n$ filling for $n > 2$ could not be analyzed in the framework of the usual analytic renormalization-group procedure.

In this paper, we present a careful numerical analysis of the one-dimensional $SU(n)$ -symmetric Hubbard model for $n = 2, 3, 4$, and 5 using the density-matrix renormalization-group (DMRG) method.¹⁰ Besides the question where the Mott transition takes place in the $1/n$ -filled model we will consider the problem of dimerization in the half-filled case, since Marston and Affleck² predicted dimerization for even n only. This is done by calculating the one-site and two-site entropies^{11,12,13,14} whose behavior may be a better indicator of where and how a quantum phase transition occurs than the study of opening of gaps, which is notoriously difficult for a Kosterlitz-Thouless transition.

The setup of the paper is as follows. The Hamiltonian is presented and the role of umklapp processes at commensurate fillings is discussed in Sec. II. A few questions concerning the numerical procedure used in the paper are presented in Sec. III. In Sec. IV, the accuracy is tested on the $SU(2)$ Hubbard model. The results obtained for half-filled and $1/n$ -filled systems for $n > 2$ are given in Sec. V and VI, respectively. The conclusions are summarized in Sec. VII.

II. THE HAMILTONIAN AND THE ROLE OF UMKLAPP PROCESSES

The Hamiltonian of the $SU(n)$ Hubbard model is written in the form

$$\begin{aligned} \mathcal{H} = & -t \sum_{i=1}^N \sum_{\sigma=1}^n (c_{i,\sigma}^\dagger c_{i+1,\sigma} + c_{i+1,\sigma}^\dagger c_{i,\sigma}) \\ & + \frac{U}{2} \sum_{i=1}^N \sum_{\substack{\sigma, \sigma'=1 \\ \sigma \neq \sigma'}}^n n_{i,\sigma} n_{i,\sigma'}, \end{aligned} \quad (1)$$

where N is the number of sites in the chain, $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) creates (annihilates) an electron at site i with spin σ , the spin index is allowed to take n different values, $n_{i,\sigma}$ is the particle-number operator, t is the hopping integral between nearest neighbor sites, and U is the strength of the on-site Coulomb repulsion. In what follows t will be taken as the unit of energy. The dimensionless U and the dimensionless gaps used in the paper are obtained by dividing their physical values by t .

The term $\sigma = \sigma'$ could have been kept in the last summation, as it is usually done in the literature, in order to display clearly the $SU(n)$ symmetry. We prefer this form where the Coulomb repulsion acts between particles of different spin index only. Since it is forbidden to have two particles of the same spin on the same site, the two expressions differ in a shift in the energy only.

At generic fillings, this model is equivalent to an n -component Luttinger liquid. It has one symmetric (charge) and $n - 1$ antisymmetric (spin) gapless bosonic modes. At special fillings, where umklapp processes may become relevant, we will be interested especially in the half-filled and $1/n$ -filled cases, gap may be opened in the spectrum of charge or spin excitations. In this section we will address the question how the charge and spin degrees of freedom are coupled by umklapp processes.

Let us consider p/q -filled systems where p and q are relative prime integers. Due to particle-hole symmetry it suffices to consider the case $p < q/2$. At such a filling the Fermi momentum is $k_F = \pi p/q$ (the lattice constant has been taken to be unity). Although the bare Hamiltonian contains two-particle scatterings only, l -particle scattering processes may appear as higher-order perturbations.¹⁵ If l particles are scattered from one of the Fermi points to the opposite one, the total change in the momentum is

$$\Delta k = \pm 2k_F l = \pm 2\pi p/q. \quad (2)$$

Such umklapp processes are allowed by momentum conservation if Δk is an integer multiple of 2π , i.e., l has to be a multiple of q . The leading, lowest-order umklapp processes correspond to $l = q$. Since the interaction is assumed to be local in real space, in the dominant umklapp processes all scattered particles have to have different spin indices, i.e., we will assume that $l \leq n$.

Since the most significant contribution to low-lying excitations comes from fermion states close to the Fermi points, a linearized spectrum is assumed. The relevance or irrelevance of umklapp processes and the coupling between different modes can then be conveniently analyzed by transforming the Hamiltonian into bosonic form.¹⁶ Using the phase field ϕ_σ for particles with spin σ , which is the sum of the phases of the right- and left-moving fermions, the l -particle umklapp processes can be represented by an effective term in the Hamiltonian which is proportional to

$$\int dx \sum_{\{\sigma_i\}'} \cos [2(\phi_{\sigma_1}(x) + \dots + \phi_{\sigma_l}(x))], \quad (3)$$

where $\{\sigma_i\}'$ indicates that all spin indices are assumed to be different.

In order to investigate the role of these processes let us introduce—in the usual way—the symmetric and antisymmetric combinations of the bosonic fields for which the term charge and spin modes, respectively, will be used:

$$\begin{aligned} \phi_c(x) &= \frac{1}{\sqrt{n}} \sum_{\sigma=1}^n \phi_\sigma(x), \\ \phi_{ms}(x) &= \frac{1}{\sqrt{m(m+1)}} \left(\sum_{\sigma=1}^m \phi_\sigma(x) - m\phi_{m+1}(x) \right), \end{aligned} \quad (4)$$

with $m = 1, \dots, n-1$.

When the band is p/n filled where p is relative prime to n , the leading umklapp term corresponds to scattering of n particles from one of the Fermi points to the opposite one. In this case, the effective term in the Hamiltonian is proportional to

$$\int dx \cos [2\sqrt{n}\phi_c(x)]. \quad (5)$$

As can be seen, this term involves the charge sector only. On the other hand, for a p/q -filled band with $q < n$, several terms may appear in (3) as leading ($l = q$) umklapp processes. When written in terms of the bosonic fields, both charge and spin modes appear in them. For example in the $SU(3)$ model, where in addition to the charge mode there are two spin modes, in the half-filled case, the contribution of the two-particle umklapp processes is proportional to

$$\begin{aligned} \int dx \left(\cos \left[\sqrt{\frac{2}{3}} (2\sqrt{2}\phi_c(x) + 2\phi_{2s}(x)) \right] \right. \\ + \cos \left[\sqrt{\frac{2}{3}} (2\sqrt{2}\phi_c(x) + \sqrt{3}\phi_{1s}(x) - \phi_{2s}(x)) \right] \\ \left. + \cos \left[\sqrt{\frac{2}{3}} (2\sqrt{2}\phi_c(x) - \sqrt{3}\phi_{1s}(x) - \phi_{2s}(x)) \right] \right). \end{aligned} \quad (6)$$

These terms are relevant and the corresponding soliton excitations couple the charge and spin modes. Therefore, gap is generated not only in the charge sector but in the spin sector as well, if $q < n$, in agreement with Refs. 2 and 7.

III. NUMERICAL PROCEDURE

A. Numerical accuracy

The numerical calculations presented in this paper have been performed on finite chains with open or periodic boundary condition (OBC or PBC, respectively) using the DMRG technique,¹⁰ and the dynamic block-state selection (DBSS) approach.^{17,18} All data shown in

the figures were obtained with OBC unless stated otherwise. We have set the threshold value of the quantum information loss χ to 10^{-5} and the minimum number of block states M_{\min} to 256. All eigenstates have been targeted independently using four DMRG sweeps until the entropy sum rule has been satisfied. The accuracy of the Davidson diagonalization routine has been set to 10^{-7} and the largest dimension of the superblock Hamiltonian was around three millions.

In the DBSS procedure the DMRG parameters are set dynamically. The maximum number of block states (M_{\max}) that our program could handle was 2500, 1500, 800, and 256 for $n = 2, 3, 4$, and 5, respectively. This determines the maximal chain length that could be treated reliably with the accuracy prescribed in terms of χ . For small U ($U < 1$), where the coherence length is large, the block entropy grows very rapidly with increasing block size and the upper cutoff on the number of block states is reached at $N \simeq 90$ for the SU(3) model and at $N \simeq 30$ for the SU(4) model. For these U values and for such chain lengths the truncation error was of the order of 10^{-6} for a few DMRG iteration steps and the absolute error of our calculation is in the range of 10^{-4} . Calculations on longer systems would give less reliable results and this imposes a serious limitation on the accuracy of the results obtained by finite-size extrapolation.

B. Detecting and locating phase transitions

The most common procedure to locate quantum phase transitions numerically is to calculate energy gaps. If the SU(n) symmetry is not broken in the ground state and the band is p/q filled, in a system with N lattice sites, the number of particles with spin index σ is $N_\sigma = Np/q$. The ground-state energy is denoted by $E_0(N)$. The spin and charge gaps corresponding to the increase of energy when changing the spin of a particle or changing the number of particles were calculated according to the formulae

$$\begin{aligned}\Delta_s(N) &= E_{+1,-1}(N) - E_0(N), \\ \Delta_c(N) &= E_{+1}(N) + E_{-1}(N) - 2E_0(N),\end{aligned}\quad (7)$$

where $E_{+1}(N)$ is the lowest energy eigenvalue of the Hamiltonian when N_σ is increased by one for a given spin, $E_{-1}(N)$ is the lowest energy when N_σ is decreased by one for a given spin, and $E_{+1,-1}(N)$ is the lowest energy when the number of particles with spin σ is increased by one while the number of particles with a different σ' is decreased by one.

Since—as will be seen—it is difficult to study numerically the closing of energy gaps for small U values, an alternative approach to study quantum phase transitions has been suggested by several groups.^{11,12,13,14} It uses the anomalies appearing in the generalized l -site entropy functions. These functions are easily accessible in DMRG and require to target the ground-state wavefunction only. Moreover, they are expected to have better finite-size scaling properties than the energy gaps.

The von Neumann entropy of a single site can be determined from $s_i = -\text{Tr} \rho_i \ln \rho_i$, where the reduced density matrix ρ_i of site i is obtained from the wavefunction of the total system by tracing out all configurations of all other sites. In a similar manner generalized l -site entropies can be calculated which are often better indicators of quantum phase transitions than the one-site entropy. In our DMRG approach, the one- (s_i) and two-site ($s_{i,i+1}$) entropies at the center of the chain, for $i = N/2$ or $i = N/2 + 1$ and the block entropy of the left half of the system (corresponding to $l = N/2$) are calculated at the end of each DMRG sweeps.

It turned out that for the SU(n) Hubbard model the same single-site entropy is obtained when it is calculated on neighboring sites in the center of the chain. The sites are equivalent. The two-site entropy $s_{i,i+1}$ is, however, different when it is considered at $i = N/2$ or $i = N/2 + 1$. An indication of the existence of bond dimer order, the breaking of translational symmetry can be obtained—as an alternative to the usual dimer order parameter—from the difference of two-site entropies,

$$D_s(N) = s_{N/2,N/2+1} - s_{N/2+1,N/2+2}. \quad (8)$$

As it has been shown in Ref. 19 and will be discussed below, usually the dimer entropy difference converges faster than the energy gap, and it may be more convenient to analyze this quantity. In the next sections, we will use D_s to study the phase diagram as a function of U .

As has been pointed out recently by two of the authors,²⁰ further information about possible nonuniform phases can be obtained from the study of the length dependence of the von Neumann entropy of a block of l sites in a finite chain, $s(l)$, $l = 0, \dots, N$, and its Fourier spectrum,

$$\tilde{s}(q) = \frac{1}{N} \sum_{l=0}^N e^{-iq l} s(l). \quad (9)$$

A finite peak at a nonzero wave vector indicates a corresponding modulation of the state. E. G., in a dimerized (trimerized) state the $q = \pi$ ($q = 2\pi/3$) Fourier component is nonvanishing. Furthermore, in a gapless model the central charge can be derived^{21,22,23,24} from the initial slope of the length dependence of $s(l)$. This can help to distinguish better gapped and gapless regimes.

C. Finite-size scaling

The large- N limit of the energy gaps and entropies can be obtained if appropriate scaling functions are used. In a critical, gapless model, in leading order, the gap $\Delta(N)$ is expected to scale to zero as $1/N$. In a non-critical model the scaling depends on the boundary condition. The leading correction is exponential, if PBC is used:

$$\Delta(N) = \Delta + c \frac{1}{N^{1/2}} \exp(-N/\xi), \quad (10)$$

while for OBC the corrections are algebraic, and $\Delta(N)$ is expected to vary as

$$\Delta(N) = \Delta + a/N^2 + \mathcal{O}(N^{-4}). \quad (11)$$

Therefore, the following fitting ansatz was used to evaluate the results obtained with OBC,

$$\Delta(N) = \Delta + a/N + b/N^2, \quad (12)$$

with Δ , a , and b as free parameters.

Local quantities, however, are expected to have a better scaling property even for OBC. For non-critical models the end effects decay exponentially with a finite correlation length, and the leading correction to the local quantities $s_{N/2}(N)$, $s_{N/2,N/2+1}(N)$, and $D_s(N)$ is expected to have the form

$$A(N) = A + dN^{-\beta} \exp(-N/2\xi), \quad (13)$$

where A is any of the local quantities listed above. This form is qualitatively similar to (10), except that $N/2$ —the distance of the middle of the chain from the boundary—appears in the exponential and the exponent of the algebraic prefactor is *a priori* unknown.

IV. THE SU(2) MODEL AS A REFERENCE SYSTEM

Since numerical accuracy and proper finite-size scaling are crucial in the present work, we have tested our approach first on the half-filled SU(2) Hubbard model, where exact results are available.

The energy of all eigenstates that have been determined using DMRG with PBC agreed up to 5 digits with the numerical solution of the Bethe-ansatz equations. The U dependence of the spin and charge gaps and the finite-size extrapolation are shown in Figs. 1 and 2, respectively.

Although the spin gap has a maximum as a function of U , this is a finite-size effect. Using (10) for the extrapolation to the thermodynamic limit, the spin gap scales to $\Delta_s = 6(1) \times 10^{-4}$ for small and large U while it is of the order of 10^{-3} in the intermediate region. Here and in what follows the digits in parentheses are the one-standard-deviation uncertainty in the last digits of the given value. The root-mean-square error (the norm of residuals) of the fit denoted by κ was 10^{-6} .

The charge gap decreases monotonically with decreasing U , and the extrapolated values obtained using (10) are finite, opening exponentially slowly,

$$\Delta(U) = a \exp[-c(U - U_c)^{-\sigma}], \quad (14)$$

which is characteristic to a Kosterlitz-Thouless transition. The non-universal constants a and c and the exponent σ were estimated together with U_c by a least square fit. The best fit with error $\kappa = 5 \times 10^{-4}$ could be achieved with $a = 100.513$, $c = 8.931$, $\sigma = 0.517$, and $U_c = 0.024$.

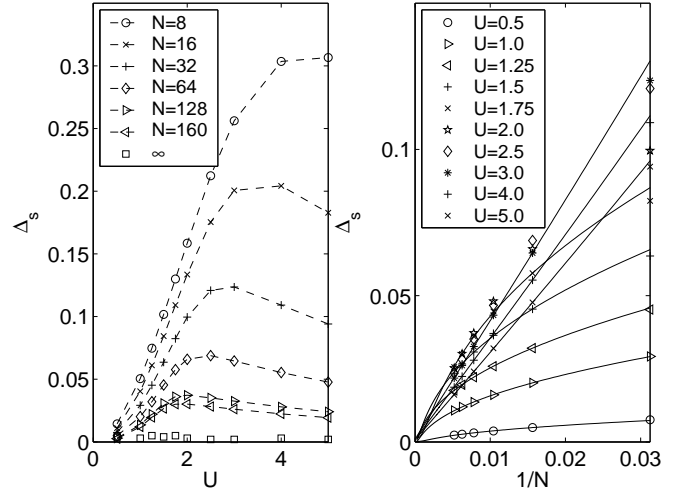


FIG. 1: U dependence and finite-size scaling of the spin gap for the half-filled SU(2) Hubbard model. The dashed lines are guide to the eye, the solid lines show the result of our fit.

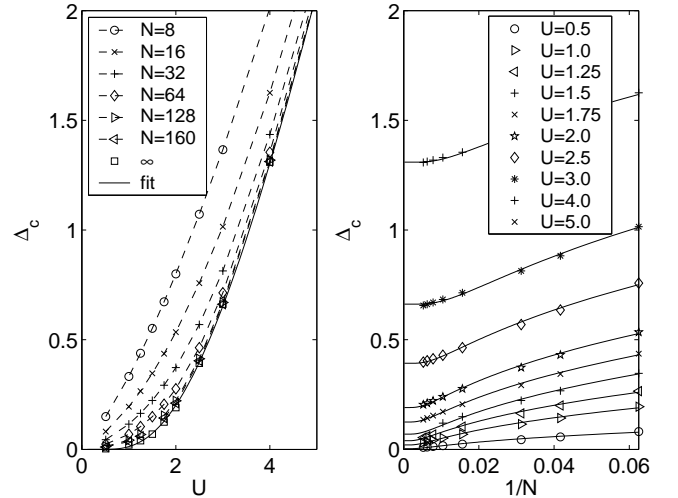


FIG. 2: U dependence and finite-size scaling of the charge gap for the half-filled SU(2) Hubbard model. The dashed lines are guide to the eye, the solid lines show the result of our fit.

If σ is fixed to $\sigma = 0.5$ the parameters a and c change only slightly, and the best fit with error $\kappa = 8 \times 10^{-4}$ gives $U_c = 0.075$. This can be taken as an indicator of the accuracy since the exact result is $U_c = 0$.

The one-site and two-site entropies measured in the middle of the chain as well as the dimerization in the two-site entropy obtained for chains with up to $N = 128$ sites as a function of U are plotted in Fig. 3. It is worth mentioning that the block entropy measured for the symmetric superblock configuration shows similar behavior as the two-site entropy.

The one-site, two-site and block entropies take their maximal value at $U = 0$, corresponding to the equipartition of local states,^{13,25} and no anomaly can be seen for $U > 0$ in agreement with the known analytic result.¹³

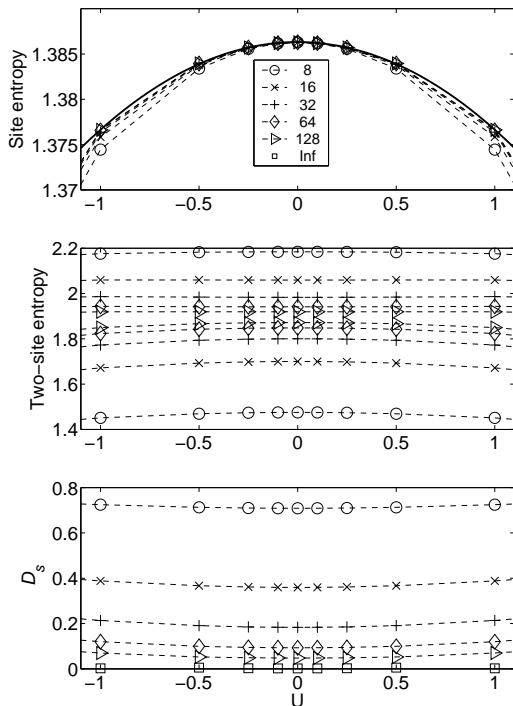


FIG. 3: One-site and two-site entropy and dimerization of the two-site entropy in the middle of the chain as a function of U for the half-filled SU(2) Hubbard model. The two sets of curves for the two-site entropy correspond to $i = N/2$ and $i = N/2 + 1$. The dashed lines are guide to the eye and the solid line is our parabolic fit.

The one-site entropy could be fitted well with a parabola

$$s_{N/2} = s_0 - AU^2, \quad (15)$$

yielding $s_0 = 1.3863$, $A = 0.009293$, with error $\kappa = 5 \times 10^{-9}$. This parabolic fit is also shown in Fig. 3. The constant s_0 and the coefficient A are in very good agreement with the exact result, $s_0 = \ln 4$ and $A = [7\zeta(3)/2\pi^3]^2/2 = 0.0092057$.

Although the two-site-entropy is markedly different on neighboring bonds in finite systems, the dimerization of the two-site entropy defined by (8) scales to $D_s = 5(1) \times 10^{-4}$ for all U , which should be considered as zero, in agreement with the known result that the SU(2) Hubbard model is not dimerized.

From these calculations we conclude that a value less than about 5×10^{-4} either for the gap or the dimerization of the two-site entropy should be taken as zero.

V. HALF-FILLED SU(n) MODELS

The renormalization-group calculations^{2,7} have shown that at half filling the charge mode is always gapped. When $n > 2$, this mode is coupled to the spin sector and this generates gaps in the spin modes, as well. Moreover, Marston and Affleck² have pointed out that for even n

the ground state is a charge-density wave state where the charge density is centered on the bonds, i.e., the system is spontaneously dimerized.

Since the arguments leading to this result cannot be straightforwardly extended to odd n we have done calculations both for even and odd n to compare the behavior of the SU(4) Hubbard model to that of the SU(3) and SU(5) models.

A. Models with even n

As has been shown, in the SU(2) model already, where relatively long chains could be studied, the energy gaps could not be determined for small U values with better accuracy than 5×10^{-4} . Since the upper cutoff on the number of DMRG block states is reached for relatively small system sizes, $N = 32$ already in the SU(4) model, determination of the $N \rightarrow \infty$ limit of the energy spectrum with the same accuracy is not possible with our computational facilities. We have calculated the energy gaps for a few large U values, where longer chains up to $N = 64$ could be treated. Although the extrapolated gaps are somewhat larger than those reported in Ref. 4, e.g., for $U = 4$ we have found $\Delta_c = 0.69(4)$ and $\Delta_s = 0.26(2)$, the results demonstrate clearly that in fact both gaps are finite.

Since our primary aim for the half-filled case was to study dimerization, we have analyzed the ground state entropy functions. The one-, and two-site entropies and the dimerization of the two-site entropy are shown in Fig. 4 for different chain lengths. While the one-site entropy shows no sign of dimerization, bond dimerization is apparent in the two-site entropy. Unfortunately the limitation for small U values discussed above applies also in the case when the extrapolated values of D_s are calculated. Although there is no doubt that D_s is finite for not too small U , and in the large- N limit, the dimerization of the two-site entropy seems to grow exponentially slowly as a function of U , resembling a Kosterlitz-Thouless transition, no reliable finite-size scaling analysis could be done to determine U_c where D_s and the energy gaps become finite. The reason is that if a smaller χ is required in the calculation for the longest chain with $N = 64$ sites, smaller D_s is obtained, thus our results shown for $N = 64$ overestimate D_s .

We try to infer U_c from the behavior of the one-site entropy. As seen, it is a continuous function of U with a maximum at $U = 0$ and without any anomaly for $U > 0$. For small U values it can be fitted well (with error $\kappa = 1 \times 10^{-7}$) by a parabola with $s_0 = 2.7723$ (the exact value is $s_0 = \ln 16$) and $A = 0.0404$.

This analytic behavior and the results obtained for the dimerization are in complete agreement with the prediction by Marston and Affleck.²

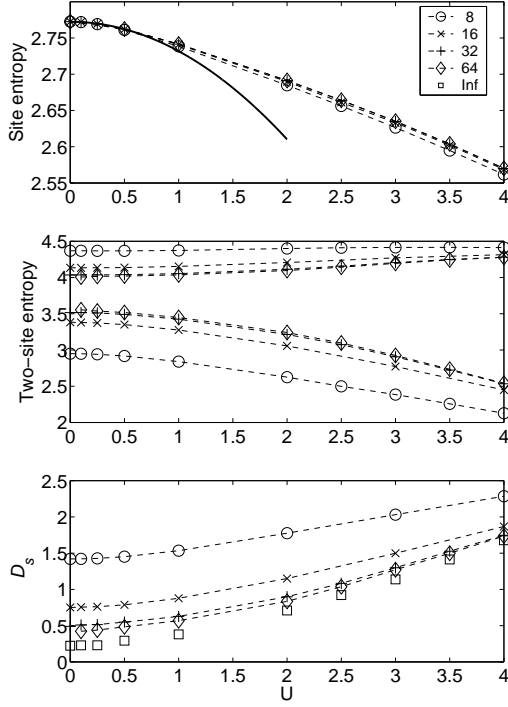


FIG. 4: Entropy functions plotted as in Fig. 3, but for the half-filled SU(4) Hubbard model.

B. Models with odd n

We will now compare the results described above with the behavior of the SU(n) model for odd n . The U dependence of the spin gap obtained by DMRG for the SU(3) half-filled Hubbard model and the finite-size extrapolation are shown in Fig. 5. The corresponding plots for the charge gaps are shown in Fig. 6.

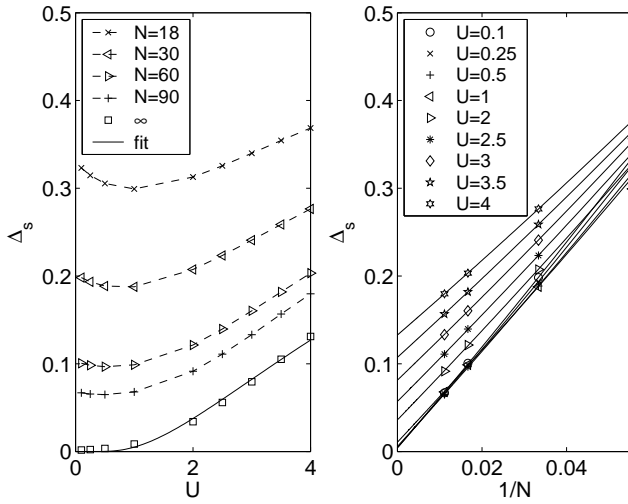


FIG. 5: The spin gap plotted as in Fig. 1, but for the half-filled SU(3) Hubbard model.

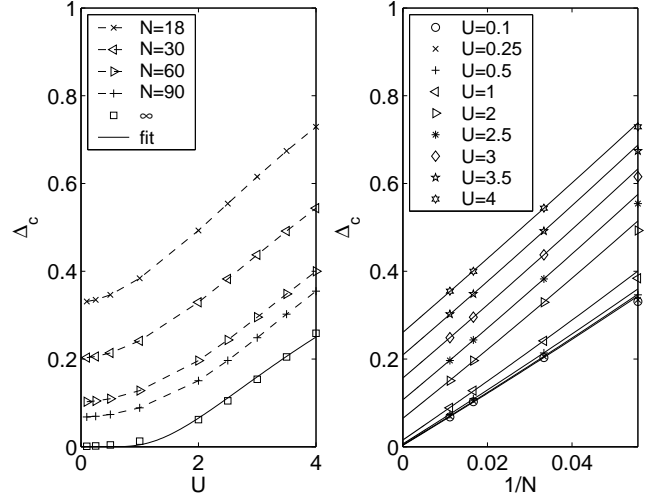


FIG. 6: The charge gap plotted as in Fig. 2, but for the half-filled SU(3) Hubbard model.

The extrapolated values obtained using (12) are summarized in Table I. They were fitted with a four-parameter curve (14). The least-square fit (also shown in Fig. 5) for the spin gap with error $\kappa = 8 \times 10^{-7}$ gives $a = 1.089$, $c = 4.9256$, $\sigma = 0.607$, and $U_c = 0.054$. When σ is fixed to $\sigma = 0.5$ we obtain $U_c = 0.098$ with error $\kappa = 2 \times 10^{-6}$.

For the charge gap the same procedure gives $a = 1.0855$, $c = 5.0492$, $\sigma = 0.9060$ and $U_c = 0.0913$ with error $\kappa = 5 \times 10^{-7}$ (this curve is also shown in Fig. 6) or $U_c = 0.099$ with error $\kappa = 2 \times 10^{-5}$ if $\sigma = 0.5$.

U	Δ_c	Δ_s
0.1	0.0010(5)	0.0017(4)
0.25	0.0016(4)	0.0021(4)
0.5	0.0040(4)	0.0035(4)
1	0.0128(3)	0.0086(3)
2	0.0618(2)	0.0339(3)
2.5	0.1047(1)	0.0559(2)
3	0.1537(2)	0.0794(2)
3.5	0.2047(1)	0.1057(1)
4	0.2586(1)	0.1318(1)

TABLE I: Extrapolated values of the spin and charge gaps in the thermodynamic limit for the half-filled SU(3) Hubbard model.

The one- and two-site entropies and the dimerization appearing in the latter one are shown in Fig. 7 for system sizes up to $N = 90$. The one-site entropy possesses a maximum at $U = 0$, and none of the entropy functions show any sign of anomaly for $U > 0$. The one-site entropy can be fitted with a parabola giving $s_0 = 2.0791$ (the exact value is $s_0 = \ln 8$) and $A = 0.0197$ with $\kappa = 5 \times 10^{-7}$. Bond dimerization is signaled again by the two-site entropy, since D_s remain finite in the large- N limit for all finite U values. Eq. (14) with fixed $\sigma = 0.5$ gives $a = 18.324$, $c = 5.827$, and $U_c = 0.013$ with error $\kappa =$

5×10^{-7} .

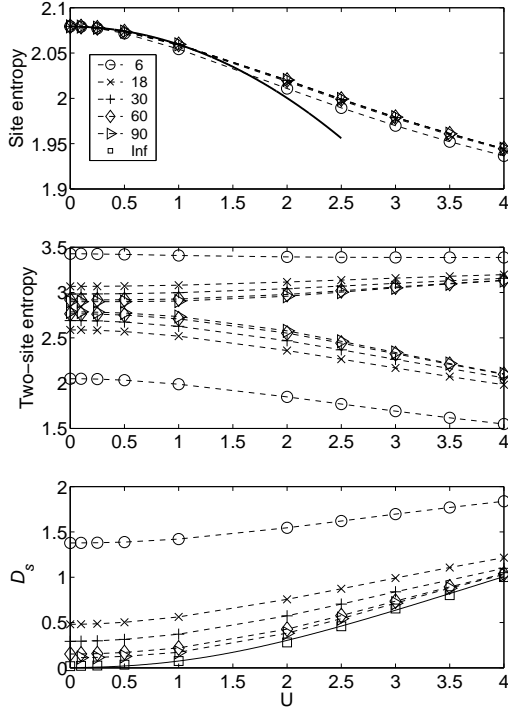


FIG. 7: Entropy functions plotted as in Fig. 3, but for the half-filled SU(3) Hubbard model.

This finding, the dimerization of the half-filled SU(3) model has been corroborated by the study of the length dependence of the block entropy. We have determined the von Neumann entropy of blocks of length l for various chain lengths and calculated the Fourier components. It was found that an oscillatory component is superimposed on the smoothly increasing $s(l)$ as l varies from $l = 0$ till $l = N/2$ (due to its definition $s(l)$ decreases for $l > N/2$ to vanish at $l = N$) and a finite Fourier component at $q = \pi$ is obtained in the $N \rightarrow \infty$ limit. This is shown in Fig. 8. Comparison to the results obtained for the half-filled SU(2) and SU(4) models, also shown in the figure, it is clearly seen that the SU(3) model behaves like the SU(4) model, both are dimerized, while the SU(2) model is not.

Due to the limitations imposed by our computing facility we could calculate the entropy functions for the SU(5) Hubbard model for chains up to $N = 20$ lattice sites only. Therefore these results show tendencies only. It was found that in the half-filled case the one-site and two-site entropies have a smooth maximum at $U = 0$ and the dimerization of the two-site entropy as a function of U as well as the oscillation of the block entropy show similar behavior as in the half-filled SU(3) and SU(4) models: it is finite, the system is dimerized.

From all these results we conclude that the half-filled SU(n) Hubbard models with odd n behave in the same way as predicted for even n .

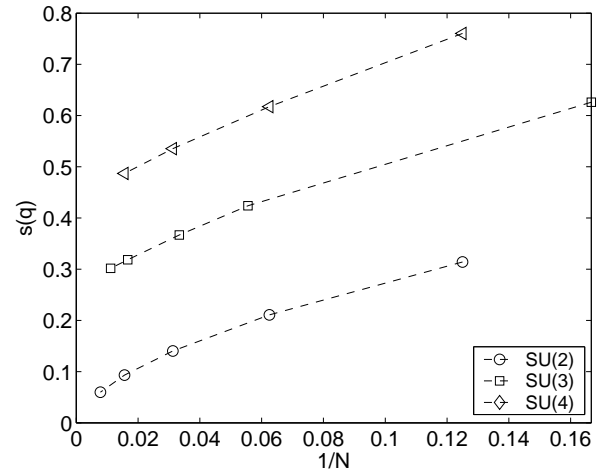


FIG. 8: Finite-size scaling of the $q = \pi$ Fourier component of the half-filled SU(n) Hubbard model for $n = 2, 3, 4$ at $U = 4$.

VI. $1/n$ -FILLED SU(n) MODELS

The other interesting situation which in a certain sense is the analogon of the half-filled SU(2) model is the $1/n$ -filled band, where the number of electrons is equal to the number of lattice sites. In this case umklapp processes in which n particles with different spin indices are scattered across from k_F to $-k_F$ (or vice versa) may become relevant. An earlier study³ of the model using both analytic and numerical quantum Monte Carlo approach suggested that the spin gap vanishes for all U , while the charge gap opens exponentially slowly for $U > U_c$ but with finite U_c . Since these numerical calculations have been performed for relatively short chains up to $N = 30$ sites, in this section we investigate in detail the same problem for the SU(3) model on longer chains using a different and hopefully more accurate procedure, and check the results for SU(4) and SU(5) models, too.

A. SU(3) model at one-third filling

The U dependence of the spin gap obtained by DMRG for the SU(3) one-third-filled Hubbard model and the finite-size extrapolation are shown in Fig. 9. The corresponding plots for the charge gaps are shown in Fig. 10.

As it is seen, for the chain lengths available the spin gap is a decreasing function of U and it scales to zero slower than $1/N$. An upper bound $\Delta_s = 0.003(2)$ is obtained for all U if (12) is used for the extrapolation. A better fit can be achieved by the ansatz

$$\Delta(N) = \Delta + a/N^b, \quad (16)$$

with the exponent b as a free parameter. This fit gives $\Delta_s = 0.0006(3)$ with b varying between 0.9 and 0.98. This difference is an indicator of the limits of our calculations. As mentioned earlier a gap 5×10^{-4} should be taken to

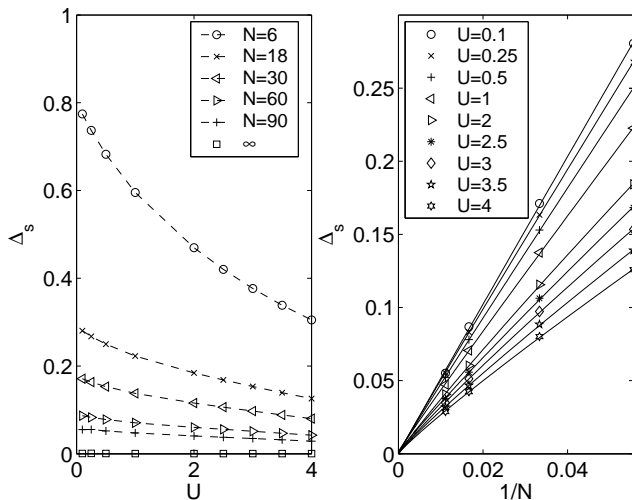


FIG. 9: Spin gap plotted as in Fig. 1, but for the one-third-filled SU(3) Hubbard model.

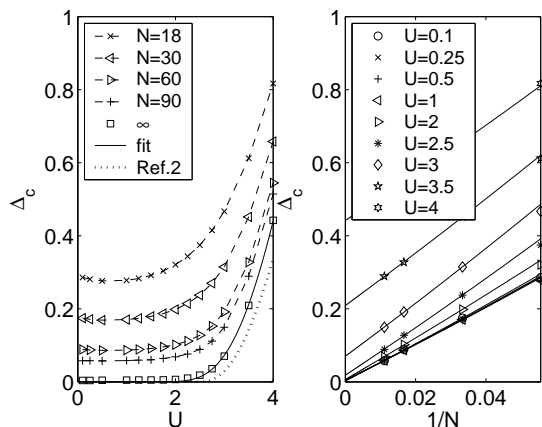


FIG. 10: Charge gap plotted as in Fig. 2, but for the one-third-filled SU(3) Hubbard model.

be zero. Thus we conclude that the spin gap vanishes in the large- N limit for all positive U .

In contrast to this, the charge gap is a monotonically increasing function of U for all finite system sizes. It scales to finite values not only if U is large enough but for small U values, as well. Our finite-size scaling analysis predicts small but finite charge gap. The extrapolated values are given in Table II. These values are larger than those given in Ref. [3] where the longest chain used in the finite size scaling analysis had $N = 30$ sites. The reason for the discrepancy is that the $1/N^2$ corrections in Eq. (11) can be seen for longer systems only. The extrapolated values were fitted with the four-parameter function (14). The best estimates for the parameters are: $a = 8.68$, $c = 28.12$, $\sigma = 1.62(3)$, and $U_c = 0.03(3)$ (this curve is also shown in Fig. 10). The error of the fit is $\kappa = 2 \times 10^{-4}$. The fit with fixed $\sigma = 0.5$ gives $U_c = 0.36$ with error $\kappa = 2 \times 10^{-3}$. These U_c values are

much smaller than the one found Ref. 3. Even though it has been emphasized in that work that the extrapolated charge gap can be fitted with U_c varying between 0 and 2.2, their best estimate was $U_c = 2.2$. The curve using their parameter values, $a = 45.050$, $c = 6.567$, and $\sigma = 0.5$ is also plotted in Fig. 10. It is clearly seen that this curve is well below our extrapolated data even for large U . The authors of Ref. [3] supported their finding by a theoretical estimate for the critical coupling U_c which they have found to be the order of unity. Our best estimate at least an order of magnitude smaller.

U	Δ_c	U	Δ_c
0.1	0.0037(4)	2	0.0065(3)
0.25	0.0039(5)	2.25	0.0101(3)
0.5	0.0043(4)	2.5	0.0183(2)
1	0.0048(4)	2.75	0.0360(2)
1.25	0.0049(4)	3	0.0702(2)
1.5	0.0051(4)	3.5	0.2090(1)
1.75	0.0053(3)	4	0.4421(1)

TABLE II: Extrapolated values of the charge gap in the thermodynamic limit for the one-third-filled SU(3) Hubbard model.

Since the numerical results on the gap do not give a definite answer whether U_c is finite or not, while Ref. 3 gives analytic arguments in favor of a finite critical value, we looked for further numerical evidence by studying the entropy functions. Our results are shown in Fig. 7. The one-site entropy possesses a maximum at $U = 0$. It shows no anomaly for $U > 0$. For small U , it can be fitted with the a quadratic U dependence with $s_0 = 1.9076$ (the exact value is $s_0 = 3 \ln 3 - 2 \ln 2$) and $A = 0.0138$ with $\kappa = 2 \times 10^{-7}$.

A somewhat different behavior is obtained when the entropy of bigger blocks are considered. This effect is most pronounced when the entropy for a block of length $l = N/2$ is considered. The block entropy as a function of the block length oscillates now with a period of three, the Fourier spectrum has a peak at $q = 2\pi/3$, however, this component vanishes in the large N limit, indicating that the system remains uniform. When the U dependence of the blocks of length $l = N/2$ is taken, this quantity, in contrast to what has been seen for the single-site entropy, does not have its maximum at $U = 0$, but at a somewhat larger value. This is seen in Fig. 12.

The accuracy, the allowed quantum information loss was $\chi = 10^{-4}$ in this calculation, which allowed us to consider chains with $N = 120$ sites, but this does not influence the shape of the curves. The location of the maximum is shifted by less than one percent. The inset in the figure shows the finite-size scaling of U_c , the location of the maximum of the curves. Similar calculation have been performed for the excited state with $N + 1$ or $N - 1$ particles. The U_c values obtained from the maximum are also shown in the inset. Extrapolation to the $N \rightarrow \infty$ limit gives a critical U_c that is smaller than 0.1. Similar result is observed for the two-site entropy. The location

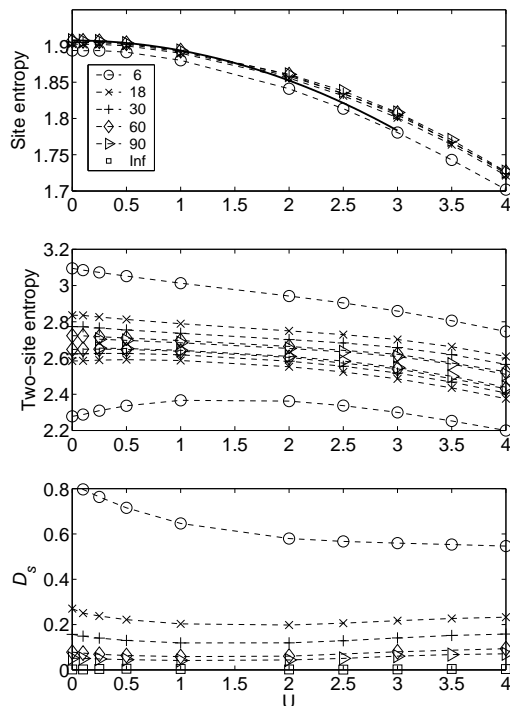


FIG. 11: Entropy functions plotted as in Fig. 3, but for the one-third-filled SU(3) Hubbard model.

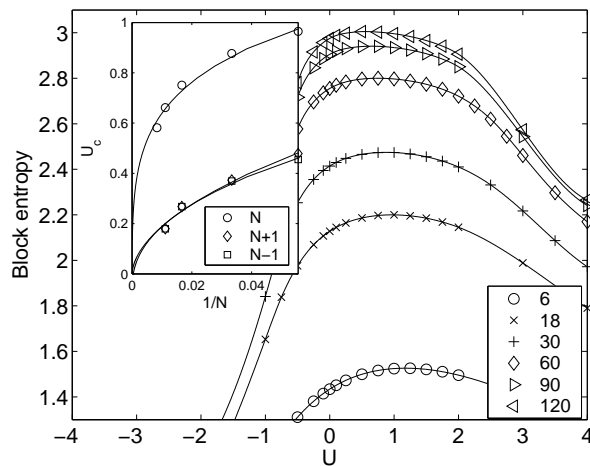


FIG. 12: Block entropy, $s(l = N/2)$, plotted as a function of U for the one-third-filled SU(3) Hubbard model. The solid lines are the result of polynomial fits. The inset shows the finite-size scaling of U_c determined from the maximum of the block entropy for the ground state as well as for excited states with $N + 1$ or $N - 1$ particles.

of the maximum shifts to $U = 0$ and the dimerization D_s vanishes for all positive U .

We have also checked the value of the central charge, which is related to the number of soft modes, using the initial slope of $s(l)$. While for $U = 0$ a value close to 3 is found, our calculation indicates that it is only 2 for $U > 0.5$. For smaller U values much longer chains would

be needed to get reliable results.

Therefore, on the basis of our numerical results we conclude that U_c is much smaller than predicted, and it could even be zero. The ground state is uniform as is the case for the half-filled SU(2) Hubbard model.

B. The SU(n) models with $n > 3$

As mentioned in Sec. III, if an accuracy $\chi = 10^{-5}$ is required, relatively short chains only could be studied for $n > 3$. For the SU(4) model we calculated the energy gaps for large U values only to compare our results with those obtained previously by quantum Monte Carlo calculation.³ Here again—similarly to what has been seen for $n = 3$ —the values obtained for the gap are somewhat larger than those reported in Ref. 3. For $U = 4$ we find $\Delta_s = 0.05(3)$ and $\Delta_c = 0.21(2)$ for the extrapolated gaps. Since this small but finite Δ_s does not allow to draw the firm conclusion that the spin gap vanishes, the entropy analysis has been performed.

The entropy functions for the quarter-filled SU(4) model show similar qualitative behavior as the half-filled SU(2) or the one-third-filled SU(3) models. The one-site entropy possesses a maximum at $U = 0$ and for small U it can be fitted with a quadratic form with $s_0 = 2.2353$ (the exact value is $s_0 = 4 \ln 4 - 3 \ln 3$) and $A = 0.138$ with error $\kappa = 3 \times 10^{-4}$. None of the entropy functions show any anomaly for $U > 0$. The dimerization of the two-site entropy seems to scale to zero, since for any U it scales to a value less than $D_s = 0.02(3)$. Although for finite systems the Fourier spectrum of the block entropy $\tilde{s}(q)$ has a peak at $q = \pi/2$, it scales to zero in the thermodynamic limit. The ground state is in fact uniform.

Due to the similarity in the behavior of the half-filled SU(2), one-third-filled SU(3), and quarter-filled SU(4) models, we suggest that—in disagreement with the result obtained by Assaraf *et al.*³ who predicted vanishing charge gap for $U < 2.8$ —the charge gap opens exponentially slowly at $U_c = 0$.

The entropy functions of the 1/5-filled SU(5) model have been calculated for chains up to $N = 30$ lattice sites only. Although no reliable finite-size scaling could be performed, our results indicate similar features as seen in the other $1/n$ -filled models. The one-site entropy possesses a maximum at $U = 0$ and it is a smooth function of U . We expect, therefore, that in this case as well the Mott transition occurs at $U_c = 0$.

VII. CONCLUSION

In summary, we have studied the one-dimensional SU(n) ($n = 2, 3, 4$, and 5) Hubbard model using the density-matrix renormalization-group method. Excitation gaps, l -site entropies, and Fourier spectrum of the block entropy have been calculated numerically. The numerical accuracy has been controlled by the quantum in-

formation loss χ which also sets a limit on the largest chain lengths whose properties could be determined with an *a priori* defined accuracy. Our method has been tested on the SU(2) Hubbard model in order to see similarities and differences when the $n > 2$ cases are studied.

First, the model at half filling has been considered. The prediction² based on a large- n analytical calculation, that the SU(n) chain is bond dimerized for even $n > 2$ has been numerically verified, and it has been shown that exactly the same behavior is found for odd n . For the half-filled models both the spin and charge excitation gaps are finite for all finite Coulomb repulsion U , and they open exponentially slowly, indicating a Kosterlitz-Thouless transition at $U_c = 0$. Since finite-size scaling is notoriously difficult in the neighborhood of a Kosterlitz-Thouless transition, we have studied the behavior of several entropy functions. They show no anomalies for $U > 0$ which also supports that $U_c = 0$. This is, however, not a usual metal-insulator transition. The dimerization for $n > 2$ has been corroborated by the peak at $q = \pi$ in the Fourier spectrum of the length dependence of the block entropy.

Next, $1/n$ -filled systems have been studied. It has been shown that the one-third-filled SU(3) model and the quarter-filled SU(4) model behave exactly in the same way as the half-filled SU(2) model. Although the length dependence of the block entropy shows a characteristic oscillation with a period of $1/n$, the corresponding Fourier components vanish in the thermodynamic limit, confirming that the ground state is spatially uniform. The spin gap vanishes while the charge gap opens ex-

ponentially slowly for $U > 0$. Moreover, the best fit gives a value for U_c that is very close to zero. The location of the transition has been checked by studying the U dependence of various entropy functions. While the one-site entropy has its maximum at $U = 0$, this is not the case for larger blocks. Nevertheless, their maximum shifts to $U = 0$ in the large N limit. Within our numerical accuracy the opening of the charge gap happens with a Kosterlitz-Thouless type transition at $U_c = 0$. The fifth-filled SU(5) Hubbard model shows similar behavior. Of course, a finite but very small $U_c < 0.1$ cannot be excluded, but even such a small value indicates that the role of higher order umklapp processes needs to be reexamined.

In a recent work,²⁶ it has been shown that the entropy profile of the SU(2) Hubbard model for different U values as a function of the band filling indicates clearly the Mott transition at half filling for any positive U . Extension of this work to SU(n) models might provide further evidence or discredit our result that in all cases studied $U_c = 0$.

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- ¹ J. Hubbard, Proc. Roy. Soc. A **276**, 238 (1963); *ibid.* **277**, 237 (1964); *ibid.* **281**, 401 (1964); *ibid.* **285**, 542 (1965).
 - ² J. B. Marston and I. Affleck, Phys. Rev. B **39**, 11538 (1989).
 - ³ R. Assaraf, P. Azaria, M. Caffarel, and P. Lecheminant, Phys. Rev. B **60**, 2299 (1999).
 - ⁴ R. Assaraf, P. Azaria, E. Boulat, M. Caffarel, and P. Lecheminant, Phys. Rev. Lett. **93**, 016407 (2004).
 - ⁵ C. Honerkamp and W. Hofstetter, Phys. Rev. Lett. **92**, 170403 (2004).
 - ⁶ F. F. Assaad, Phys. Rev. B **71**, 075103 (2005).
 - ⁷ E. Szirmai and J. Sólyom, Phys. Rev. B **71**, 205108 (2005).
 - ⁸ E. Szirmai and J. Sólyom, Phys. Rev. B **74**, 155110 (2006).
 - ⁹ E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).
 - ¹⁰ S. R. White, Phys. Rev. Lett. **69**, 2863 (1992); Phys. Rev. B **48**, 10345 (1993).
 - ¹¹ P. Zanardi, Phys. Rev. A **65**, 042101 (2002).
 - ¹² L.-A. Wu, M. S. Sarandy, and D. A. Lidar, Phys. Rev. Lett. **93**, 250404 (2004).
 - ¹³ S.-J. Gu, S.-S. Deng, Y.-Q. Li, and H.-Q. Lin, Phys. Rev. Lett. **93**, 086402 (2004).
 - ¹⁴ Ö. Legeza and J. Sólyom, Phys. Rev. Lett. **96**, 116401 (2006).
 - ¹⁵ T. Giamarchi and A. J. Millis, Phys. Rev. B **46**, 9325 (1992).
 - ¹⁶ For a review, see, e.g., J. Sólyom, Adv. Phys. **28**, 201 (1979); and A. O. Gogolin, A. A. Nersisyan, A. M. Tsvelik, *Bosonization and Strongly Correlated Systems* (Cambridge University Press, Cambridge, 1998).
 - ¹⁷ Ö. Legeza, J. Röder, and B. A. Hess, Phys. Rev. B **67**, 125114 (2003).
 - ¹⁸ Ö. Legeza and J. Sólyom, Phys. Rev. B **70**, 205118 (2004).
 - ¹⁹ K. Buchta, G. Fáth, Ö. Legeza and J. Sólyom, Phys. Rev. B **72**, 054433 (2005).
 - ²⁰ Ö. Legeza, J. Sólyom, L. Tincani and R. M. Noack, cond-mat/0610499 (2006).
 - ²¹ C. Holzhey, F. Larsen, and F. Wilczek, Nucl. Phys. **B424**, 443 (1994).
 - ²² P. Calabrese and J. Cardy, J. Stat. Mech.: Theor. Exp. P06002 (2004).
 - ²³ I. Affleck and A. W. W. Ludwig, Phys. Rev. Lett. **67**, 161 (1991).
 - ²⁴ N. Laflorencie, E. S. Sorensen, M-S Chang and I. Affleck, Phys. Rev. Lett. **96**, 100603 (2006).
 - ²⁵ D. Larsson and H. Johannesson, Phys. Rev. Lett. **95**, 196406 (2005).
 - ²⁶ V. V. Franca and K. Capelle, (unpublished, cond-mat/0605207).